netlognews

NETL's R&D newsletter

January 2010, Issue 16

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U.S. DEPARTMENT OF ENERGY | the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

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ON THE COVER

Ultra-deep Drilling Simulator pressure vessel withstands extreme pressures up to 30,000 psi.

netlog is a quarterly newsletter, which highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.

NETL Director to Retire

On December 14th, the U.S. Department of Energy (DOE) announced that Carl O. Bauer is retiring from federal service and leaving the National Energy Technology Laboratory (NETL) effective February 28, 2010, following a distinguished, four-year tenure as the laboratory's director, completing an impressive federal civilian and military career.

Bauer was appointed NETL Director in August 2005 after serving as NETL Deputy Director, Director of NETL's Office of Coal and Environmental Systems, and Director of NETL's Office of Product Management for Environmental Management. Under his leadership, the laboratory expanded its international outreach and collaboration, strengthened its role as the key national laboratory addressing the challenges of producing and using fossil energy, and extended its expertise into new areas of investigation, such as electricity delivery and more energy-efficient buildings, appliances, and vehicles.

In 2007, Bauer received the prestigious Laboratory Director of the Year award from the Federal Laboratory Consortium for Technology Transfer and was the sole recipient of the Washington Coal Club's Annual Achievement Award for significant leadership and contributions in the energy arena.

Bauer will continue as NETL Director until December 31, 2009, at which time he will be detailed to the U.S. DOE's Office of Fossil Energy headquarters in Washington, D.C., where he will advise on strategic planning. Dr. Anthony Cugini, current Director of NETL's Office of Research and Development, will serve as Acting Director effective January 1, 2010.

A national search is being initiated to find Bauer's replacement as NETL Director.

Extreme Drilling Laboratory Announces Debut of Ultra-deep Drilling Simulator

The Extreme Drilling Laboratory (XDL) proudly announces the much-anticipated debut of its prototype Ultra-deep Drilling Simulator (UDS), the rock star of the XDL. Drilling research will begin soon at an experimental well site with pressures reaching 30,000 pounds of force per square inch and temperatures exceeding 480 °F at the bottom of the well. One of the many unique features of this extreme drilling research is that 100 percent of the drilling will occur above ground. In addition, the UDS operating pressure and temperature ranges are three times greater than those found in similar drilling rigs and are representative of conditions found in ultra-deep wells, or wells with depths near 30,000 feet.


The Extreme Drilling Laboratory is located at the NETL Morgantown site. Initial research operations will begin in 2010.

The concept of the high-tech facility located in Morgantown, W.Va., was conceived in cooperation with industry and funded by the federal government under Section 999 of the Energy Policy Act of 2005. Research conducted in the XDL is expected to have a direct impact on increasing our domestic supply of oil and natural gas by developing affordable, efficient, and environmentally safe means to harvest ultra-deep oil and natural gas resources.

Contact: William Ayers, 304-285-4125

Hybrid Technology Response Modeled to Changes in Power Demand

One of the most critical problems that must be addressed in gas turbine-fuel cell hybrid technology is temperature control. A hybrid system designed to operate efficiently for a given base load may not easily accommodate peak loads. Using ASPEN PLUS® simulation software with special modules to calculate fuel cell performance, NETL scientists have modeled a simple hybrid system configuration consisting of a standard solid oxide fuel cell and a single compressor-turbine pair to determine the effects of key configuration parameters on system temperature. Results of scaling the configuration model over a range of fuel input and power output are discussed in an article entitled "Scaling a Solid Oxide Fuel Cell Gas Turbine Hybrid System to Meet a Range of Power Demand" in the *Journal of Fuel Cell Science and Technology*, a quarterly publication of the American Society of Mechanical Engineers (Vol. 7 (2010), No. 1, Article 015001).

Contact: John VanOsdol, 304-285-5446

NETL Study Examines Convection-Radiation Heat Transfer in Nonlinear Fluid

NETL scientists have studied fully developed flow down an inclined plane for a generalized second-grade fluid where viscosity is a function not only of shear rate (shear-thinning or shear-thickening) but also of temperature. NETL researchers have formulated constitutive relations and have numerically simulated a variety of engineering problems dealing with complex materials such as drilling fluids, powders, and suspensions.

Free surface flow problems are an engineering challenge, and combined convection-radiation at boundaries has major applications in many industries. Results of the study appear in *Mathematical Problems in Engineering* (Vol. 2009, Article 232670).

Contact: Mehrdad Massoudi, 412-386-4975

Smoldering combustion of coal.

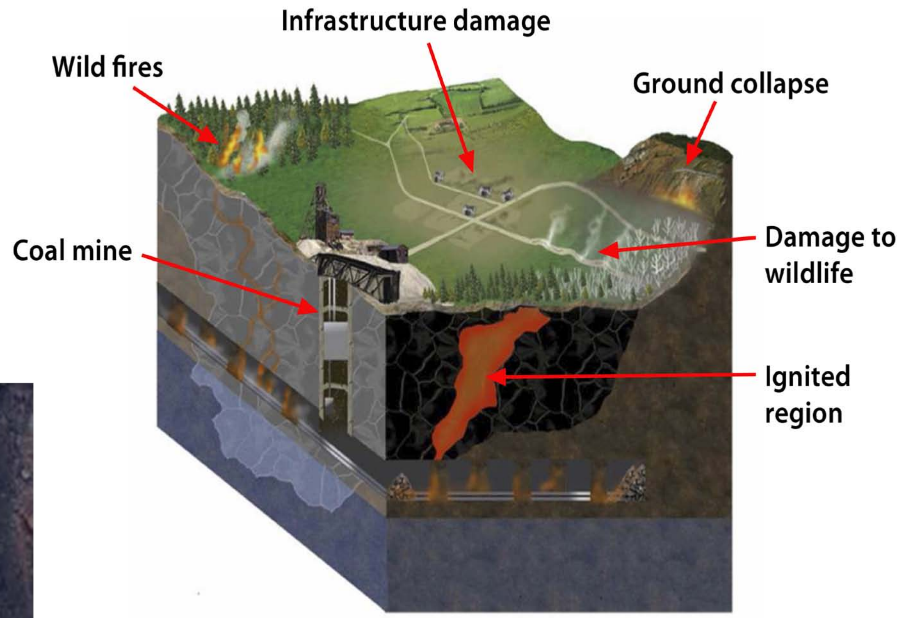


Illustration by Rori Haden and Guillermo Rein, University of Edinburgh

Illustration above shows how an underground fire can be visualized as a sequence of ignitions and what occurs as a result.

Underground Coal Fires

Underground coal fires represent a substantial nuisance in terms of property damage, public safety, greenhouse gas generation, and coal resource destruction. Many underground coal fires burn throughout the world, with some of these fires burning for decades or even longer. They are very difficult to extinguish and generate much carbon dioxide, while squandering valuable land and coal resources. The emissions of carbon dioxide, mercury, and noxious gases from these fires are significant. It is estimated that these fires generate as much as 3 percent of the world's annual carbon dioxide emissions and consume as much as 5 percent of its mineable coal.

Some of the techniques employed to combat, detect, and monitor these fires were illustrated in a presentation at the 26th International Pittsburgh Coal Conference in September 2009.

Professor Ali Rangwala, from the Department of Fire Protection Engineering at Worcester Polytechnic Institute, co-authored the paper.

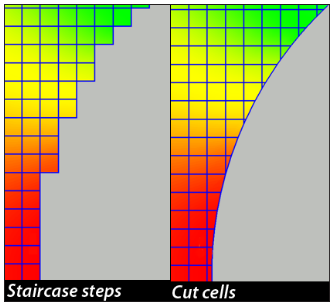
The possibility of using large amounts of carbon dioxide for fighting these fires, halting or slowing the generation of greenhouse carbon dioxide gas, and recovering useful fuel gas, was also discussed. The mechanisms by which the fires start and spread were briefly detailed as well.

Here is a fact sheet created by the U.S. Geological Survey describing underground coal fires and their impact on the environment.

Contact: Evan J. Granite, 412-386-4607

Improved Multiphase Flow Solver Released

The Cartesian grid cut-cell technique has been implemented in MFIX (Multiphase Flow with Interphase eXchanges). This new capability allows the definition of curved or sloping boundaries, instead of the usual stair-step representation. Computational cells are truncated at the wall to conform to the shape of the boundaries. Multiphase flows over complex 2D or 3D geometries can now be simulated with better accuracy. Results obtained with the new cut-cell technique show a clear improvement over the usual stair-step method. Fairly coarse grids can be used with the new cut-cell technique, which reduces the computational time required to obtain the flow solution. The Cartesian grid technique is available for the Eulerian-Eulerian approach and includes no-slip and free-slip boundary conditions for either gas or solids phases. MFIX is an open-source software developed at NETL, and the latest version of the code is now available to the MFIX community.



The image shows the difference in the computational mesh between the original stair-step method and the new cut-cell technique for a sloping wall.

Contact: Chris Guenther, 304-285-4483

NETL Measures Conversion Indices for Coal Size and Density Fractions

NETL researchers conducted tests at high temperature (1600 ° C) and high pressure (3 MPa) in a lab-scale pressurized premixed pulverized coal reactor to validate the coal conversion and particle size changes during gasification. The conversion index for each of the final products was determined, and influences of size and density were found to be insignificant compared to the severity of process. This knowledge is being integrated with particle trajectories from fluid dynamic models to evaluate the extent of flyash formation from each of the coal size and density fractions.

Contact: Larry Shadle, 304-285-4647

Technique Patented to Optimize Catalyst Size for Chemical Reactors

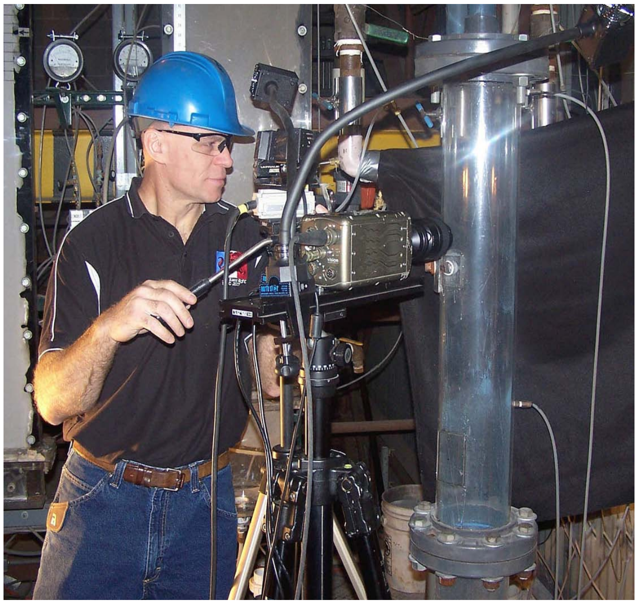
A U.S. patent was recently granted for a technique to systematically predict the optimum particle size for hydrocarbon-producing reactors. The technique uses multiphase computational fluid dynamics. Worldwide energy industries use various ad-hoc methods to estimate the optimum catalyst size. The NETL technique has been successfully applied to determine the optimum catalyst size of 60-70 microns for methanol production from synthesis gas in a slurry bubble column reactor. The lead inventor is Dr. Isaac K. Gamwo from NETL, and the co-inventors are former NETL research associates Professor Dimitri Gidaspow at IIT, Chicago, and Dr. Jonghwun Jung at POSCO, Seoul, South Korea.

Contact: Isaac K. Gamwo, 412-386-6537

High Speed Particle Imaging Technology Extended to Energy and Medical Applications

Scientists have developed a unique high-speed particle imaging (HSPI) system now in demand for many applications, including industrial and medical uses. The HSPI system produces valuable data due to the development of particle recognition and tracking software.

In recent months, the HSPI system was applied to study several industry research units at Particulate Solids Research, Inc., (PSRI) an industrial research organization in Chicago, IL., and is currently being applied to study hemodynamics (blood flow) in an oxygenator catheter that functions as an artificial lung at the University of Pittsburgh's McGowan Institute for Regenerative Medicine. HSPI is an excellent tool for studying hemodynamics because blood is similar to energy flow fields in that blood flow is a mixture of a fluid and a high concentration of particles (blood cells).



Roy Hayes, senior research engineer at Particulate Solids Research, Inc., applies NETL's high- speed particle imaging system to study cluster phenomena at one of PSRI's research units in Chicago.

PSRI is a research consortium of 30 major chemical and energy companies. The studies at PSRI included measurement of particle clustering phenomena under industrially relevant conditions. Particle clustering can dramatically change the performance of processes based on particle dynamics. Fifty percent of all industrial chemical-processing units rely on particle dynamics.

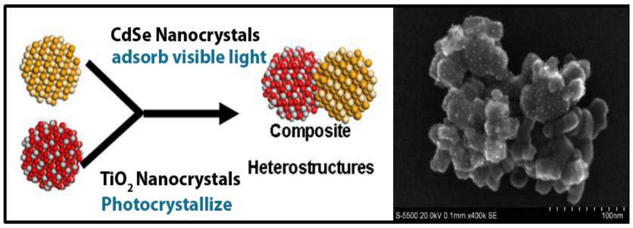
With NETL's HSPI system, particle clustering was observed for the first time in a fluidized bed. Three papers have been written and submitted to journals and conferences on the particle clustering study.

The HSPI system is also being applied to study numerous experiments at NETL. In NETL's Cold Flow Circulating Fluidized Bed unit, more than 10 conditions that simulate various gasifier phenomena were studied with the HSPI system during the past few months. The HSPI system is producing new views of particle phenomena in simulated gasifier flow fields.

Other projects ongoing at NETL using the HSPI system include a novel table feeder for biofuels, a chemical looping demonstration unit, and an experiment to study particle-wall interactions in combustors.

Plans are underway to apply the HSPI system to visualize drill tip behavior inside NETL's 30,000 psi ultra-deep drilling experiment (*see article this issue page 3*).

Contact: Frank Shaffer, 412-386-5964



(Left panel) Schematic diagram of the new photocatalytic technology for converting CO_2 into fuels. (Right panel) SEM image of a heterostructured CdSe/Pt/TiO_2 photocatalyst synthesized and tested by the NETL team (scale bar 100 nm).

Promising New Photocatalyst Developed for CO_2 Reuse

A new photocatalyst has been developed that is capable of using the low-energy, visible light portion of the electromagnetic spectrum for converting carbon dioxide (CO_2) and water (H_2O) into methane, methanol, and other value-added chemicals. The catalyst is believed to be the first of its kind for this process. A manuscript detailing this new photocatalyst was published in the *Journal of Physical Chemistry Letters* (C. Wang, R. Thompson, J. Baltrus, C. Matranga, *J. Phys. Chem. Letters*, Vol 1, pgs 48-53), and a provisional patent application also has been filed on the technology.

The catalyst combines a cadmium selenide (CdSe) nanocrystal photosensitizer with titania (TiO_2) to create a heterostructured catalyst capable of utilizing the visible portion of the electromagnetic spectrum for CO_2 reuse applications.

In this system, the CdSe nanocrystals absorb visible light photons creating excited electrons, which are injected into the TiO_2 to reduce CO_2. The photoactivity of this system can be systematically tuned to utilize different regions of the electromagnetic spectrum just by changing the size of the nanocrystal photosensitizer.

Previous uses of unsensitized TiO_2 for this application have had limited utility because the large band gap of TiO_2 requires high-energy, ultraviolet excitation to initiate photocatalytic processes. Since ultraviolet light makes up only approximately 1 to 5 percent of the total sunlight reaching the earth's surface, these unsensitized TiO_2 catalysts do not fully utilize the solar spectrum.

The visible light activity of the catalysts developed at NETL represents a significant advance in the development of new technologies for CO_2 capture and reuse.

Contact: Christopher Matranga, 412-386-4114

New Option for Sequestration of CO_2

Researchers from NETL have developed a novel concept to neutralize caustic industrial waste material through reaction with acidic oil and gas field wastewater brines. The process results in carbonation, with CO_2 dissolved in mixtures of by-product and saline waste water.

NETL is studying the long-term storage of CO_2 underground in various geological formations. These formations offer high storage capacities. Other options for CO_2 sequestration could be considered, including the use of caustic industrial waste by-products with high calcium and magnesium contents.

NETL conducted exploratory studies to determine the CO_2-bearing capacity of reactive mixtures of brine with three caustic industrial by-products: flue gas desulfurization spray dryer ash, Class C fly ash sub-bituminous coal combustion by-product, and bauxite residue slurry from the alumina-production process.

Preliminary results indicate that the use of caustic industrial by-products/brine mixtures to capture and store CO_2 can serve not only to help mitigate the impact of anthropogenic CO_2 on global warming, but also to achieve neutralization of the caustic industrial waste for safe storage.

This study was published in *Environmental Engineering Science*, vol. 26, No. 8. pp. 1325-1333, 2009.

Contact: Yee Soong, 412-386-4925

Labs Host National Geographic's JASON Argonauts

Cathy Summers, NETL geologist, shows the rock collection to the Argonauts.

National Geographic's JASON Project team brings together 'Argonauts' from all over the world; three students, a middle school teacher, and a film crew visited NETL laboratories in Albany, OR, and Pittsburgh, PA. The National Geographic Society initiated the JASON Project to excite middle school children about science by participating in inquiry-based science.

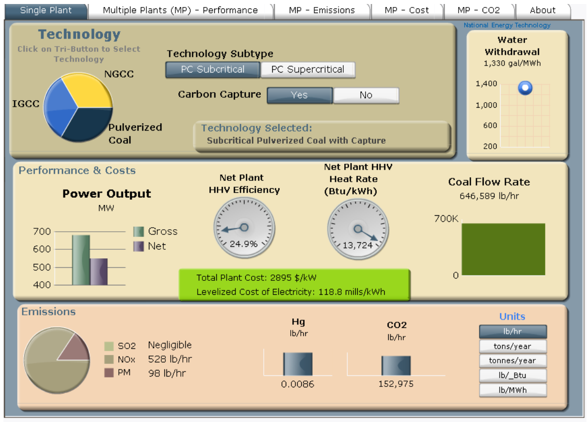
The first team visited the Albany laboratory to see NETL's world-class rock and mineral collection. The team met with researchers Cathy Summers and Bill O'Connor, who talked with them about the formation of rocks and minerals and geologic sequestration, including high-pressure experiments being done at Albany to study whether CO_2 injected deep underground will leak back out.

Dr. George Guthrie, Focus Area Leader for Geological and Environmental Systems at NETL, served as host researcher to another team during the Pittsburgh visit. As host researcher, Guthrie took the students to an underground coal mine to explore the stratigraphic features of the earth and the properties of coal. Guthrie then explained how core samples from deep under the surface of the earth can be obtained and analyzed. The students then explored the flow of fluid through a porous rock (with Dr. Grant Bromhal), simulating CO_2 sequestration. The JASON team experienced a wide range of examples of how to study earth materials from a large contingent of NETL researchers.

JASON immerses students in the mission theme by framing each curriculum around five core elements delivered via print, video, HTML, and interactive games. The core elements are (1) meet the researchers; (2) an invitation to join the mission team - mission objectives; (3) mission briefing; (4) mission labs - what science knowledge is required and why; and (5) field assignments. The resulting curriculum will be available through print, video, games, and online resources to tens of thousands of teachers and millions of students not just in the United States, but worldwide.

Contact: George Guthrie, 412-386-6571

Interactive Tool Available to Compare Plant Cost and Performance Data



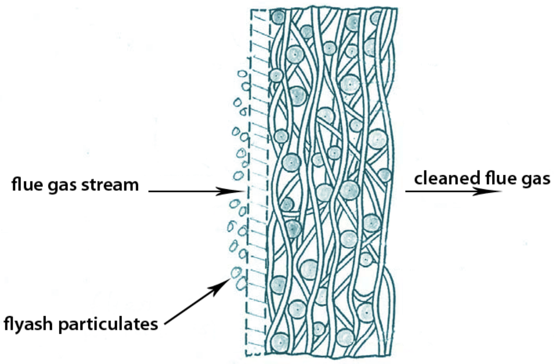
The Bituminous Baseline Performance and Cost Interactive Tool illustrates key data from the "Cost and Performance Baseline for Fossil Energy Plants - Bituminous Coal and Natural Gas to Electricity" report. This tool provides an interactive summary of the full report and serves as an electronic desk reference for quickly obtaining plant cost and performance data and for comparing and contrasting several technologies. Here is the documentation for using the tool.

This tool and the full report evaluate 12 cases for electricity production from fossil fueled plants. Performance, emissions and cost data presented include: net and gross output; heat rate; efficiency; water use; SO_2, NO_x, CO_2, PM, and Hg emissions; total plant cost; and levelized cost of electricity.

Contact: Erik Shuster, 412-386-4104

Patented Mercury Capture Method Successful in Bench Tests

Applying a novel approach that employs sorbent particles embedded in commercial bag house fabric material, NETL researchers have demonstrated a capture rate greater than 90 percent for mercury contained in a flue gas slipstream from a 500-lb/hr pulverized coal-fired combustion unit. The novel concept is readily adaptable to any gas treatment system that already employs a bag house for particulate control. In principle, pollutant-specific sorbent materials can be incorporated into the fabric, not only for mercury capture, but also for mercury oxidation in situations where a downstream wet scrubber is available. The approach avoids cross-contamination of fly ash by activated carbons and mercury, which adversely affect its suitability for use as a concrete amendment. It also extends to the cleanup of aqueous waste streams and syngas when sorbent and supporting membrane are compatible with process conditions.



Schematic of particle-loaded membrane.

Contact: Edgar Klunder, 412-386-4678

New Capability for Fuel Cell Materials Characterization

A research team from NETL and West Virginia University has developed a new experimental capability and mathematical analysis method for electronic conductivity relaxation (ECR) material characterization.

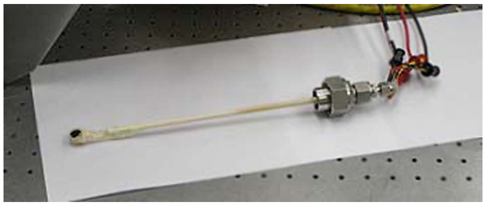
The ECR technique will be used to obtain data on two of the most important properties for solid oxide fuel cell cathodes, the surface oxygen exchange rate and oxygen bulk diffusion coefficients of mixed electronic and ionic conductors.

Compared with other techniques used to obtain the same results such as the isotope exchange depth profile method, ECR is easier to apply and offers significant cost advantages.

Recent validation experiments measuring the conductivity of a lanthanum strontium cobalt ferrate cathode material showed good agreement with literature reported values. At present, measurements are being taken to investigate the effect of different oxygen partial pressures on these two parameters.

The ECR method will next be applied to characterize other materials of interest in NETL's infiltration approach to advance cathode stability and voltage performance.

Contact: Randall Gemmen, 304-285-4536



The electronic conductivity relaxation sample holder used for material characterization.

Potential Uses for Carbon Dioxide Captured from Coal-Burning Power Plants

The talk "Survey of Potential Uses for Carbon Dioxide Captured from Coal-Burning Power Plants" was presented to the 26th International Pittsburgh Coal Conference. The current demand for carbon dioxide is much less than 2 billion tons per year, and the idea behind carbon dioxide utilization is to put a small fraction of the carbon dioxide captured from the power plants to good use. Some of the current uses for carbon dioxide include fire suppression, food preservation, refrigeration/cooling, beverage carbonation, welding, enhanced oil recovery, coal bed methane recovery, supercritical cleaning, biomass production, and polymer-plastic manufacture. Projected future uses for carbon dioxide include producing fuel, i.e., methane and methanol; manufacturing pharmaceutical chemicals; oxy-combustion of coal; neutralizing industrial alkaline wastes; and deploying to put out large underground coal fires.

Issues in the utilization of carbon dioxide captured from power plants include the location of the power plant and utilization project, the distribution and transport of the CO_2, and the purity required for the CO_2 application. Potential future uses for carbon dioxide are in the manufacture of plastics; combined coal mine fire suppression and gasification; catalytic synthesis of fuels; and producing synthetic fuels from algae.

Contact: Evan Granite, 412-386-4607

SOFC Testing Completed at NCCC/PSDF Facility

The NETL mobile solid oxide fuel cell (SOFC) test stand – the Multi-Cell Array – was recently operated at the Wilsonville, Alabama's National Carbon Capture Center/Power Systems Development Facility to evaluate the effects of trace contaminants from coal syngas on the SOFC anode performance. Twelve cells were initially operated on coal syngas at staggered load conditions with three cells demonstrating power densities as high as 250 mW/cm^2. The 450-hour continuous test was terminated at the conclusion of gasifier operation with eight cells completing the entire test, some with power densities remaining as high as 230 mW/cm^2. In total, the system generated over 4500 cell-hours of test data and over 1 kW of total power. Post-operational microscopy will be performed to investigate mechanisms of degradation including formation of secondary anode phases and deposition of trace material. Complete results will be reported in a published research paper.

Contact: Kirk Gerdes, 304-285-4342

Article Describes Role of SOFC in Future Power Systems

NETL researchers published an article on the role of solid oxide fuel cells in advanced hybrid power systems of the future in the fall issue of Interface, a preeminent publication of the Electrochemical Society. The article was one of only four contributions that were selected for inclusion in the fall issue, which focused on the topic of solid oxide fuel cells research. The authors reported NETL research regarding the high efficiency of fuel cell-based hybrids and described the unique flexibility of hybrid systems demonstrated in tests conducted last summer using the Hybrid Performance (Hyper) project facility. Interface reaches over 10,000 targeted readers worldwide in the fields of electrochemical and solid state science and technology.

Contact: David Tucker, 304-285-4182

First SECA-Stack Test Performed

NETL has established a new capability to test solid oxide fuel cell stacks. This new capability will allow the evaluation of stack-related technology solutions for such things as gas seals, electrical contact pastes, interconnects, and flow passage designs. The first test of the system began in September 2009. The system continued to operate very well (2 amps at 0.8 volts) after about 400 hours of steady operation. In the next phase of testing using the same stack fixture, a bio-based diesel fuel will be reformed and the syngas will be passed to the stack fixture. The long-term outcome of having this capability will be to allow NETL researchers to install and operate research stacks into our hybrid research facility being used to identify viable control methods that allow DOE to achieve its high efficiency coal-based power generation target of 60 percent without CO_2 capture.

Contact: Randall Gemmen, 304-285-4536

NETL Researchers Developing Energy Storage Materials for Smart Grid

NETL researchers are developing novel, safe, environmentally benign, solid-state cathode energy storage materials that are based on sodium ion chemistry. Sodium is abundant and can be used to store large amounts of electricity cheaply, which is essential for development of the modern grid as well as for enhancing distributed power from renewable energy sources. The ion batteries work by conducting sodium ions between the cathode and the anode during charge and discharge cycles; an electrolyte serves as the migration pathway to move those ions. For larger utility scale batteries, sodium represents a significantly cheaper alternative to energy storage than lithium. This research will address the developmental gaps that exist in low cost energy storage material technology at the utility scale.

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